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United Kingdom Atomic Energy Authority
REACTOR GROUP

WINFRITH NUCLEAR DATA GROUP NOTES ON TOPICS
IN NUCLEAR DATA EVALUATION, 1964-8

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1968

000263

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ABSTRACT

This memorandum collects together a selection of brief notes written, during the course of the past few years, by the members of the Nuclear Data Group at the A.E.E., Winfrith. Many of the notes were tentative in nature and of ephemeral interest only, but it is felt that those presented here may have a wider interest to the fraternity of evaluators.

A.E.E.
Winfrith

May, 1968

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CONTENTS

WINDG NO.		Page
4	SPECIFICATION FOR REPORTS ON EVALUATION OF NEUTRON CROSS-SECTION DATA IN THE RESONANCE REGION. (Story J. S., Dec. 1964)	1
21	THERMAL NEUTRON CAPTURE CROSS-SECTIONS OF NATURAL NICKEL AND OF ITS ISOTOPES. (Story J. S., Oct. 1965)	6
25	THE ESTIMATION OF THE MEAN SPACING BETWEEN RESONANCES. (James M. F., June 1966)	10
28	INELASTIC AND COMPOUND ELASTIC NEUTRON SCATTERING BY Fe57 IN THE RANGE FROM 0 to 1 MeV. (Story J. S., Sept. 1966)	16
30	THE DOPPLER BROADENING OF NEUTRON CROSS-SECTIONS. (James M. F., Oct. 1966)	
33	Q-VALUES FOR NEUTRON INDUCED REACTIONS IN IRON. (Story J. S., Dec. 1966)	25
38	NOTE ON THE THERMAL NEUTRON ABSORPTION CROSS-SECTION OF BERYLLIUM. (Story J. S., Feb. 1967)	26
40	NOTE ON THE SLOW NEUTRON ABSORPTION CROSS-SECTIONS OF OXYGEN AND ITS STABLE ISOTOPES. (Story J. S., March 1967)	29
43	RADIATION ENERGIES OF SOME FISSION PRODUCTS: Rh106, Ba137m, Pr144. (Story J. S., May 1967)	32
44	A THEOREM CONCERNING THE MAXWELLIAN AVERAGE AND WESTCOTT g-FACTOR OF A DOPPLER BROADENED NEUTRON CROSS-SECTION, AND ITS CONSEQUENCES. (James M. F., May 1967)	34
45	INELASTIC SECONDARY ENERGY DISTRIBUTIONS FOR OXYGEN. (Story J. S., May 1967)	37
47	THE RESONANCE CAPTURE INTEGRAL OF MANGANESE. (Story J. S., June 1967)	45
51	NOTES ON THE SPECIFIC ALPHA ACTIVITY AND HALF-LIFE OF U233. (Story J. S., Oct. 1967)	47
53	ESTIMATION OF ERRORS ARISING FROM TABULAR REPRESENTATION OF THERMAL MAXWELLIAN AND FISSION NEUTRON SPECTRA IN GALAXY. (James M. F. & Story J. S., Jan. 1968)	50
57	THE DOPPLER BROADENING OF A CONSTANT CROSS-SECTION. (Story J. S., April 1968)	58

SPECIFICATION FOR REPORTS ON EVALUATION OF
NEUTRON CROSS-SECTION DATA IN THE RESONANCE REGION

1. Ideally the aim of an evaluation should be rather ambitious; to combine theory and experimental data so as to be able to answer all reasonable questions on the neutron cross-sections of the material in the resonance region, whether experimental data are available or not, to whatever accuracy is available. In Section 2 below are listed a fairly comprehensive set of the topics which might be discussed in reporting an evaluation.

For practical reasons it is often not worth while to explore every one of these topics in detail, because time may not permit an exhaustive study or because it may be known that better experimental data will soon be available. The evaluator is expected to exercise good judgement on this matter, and should therefore use the following list with discretion.

2. Items which might be discussed in an ideal evaluation report:
 - (i) Isotopic composition of the material studied.
 - (ii) Exact mass of atom or molecule of the material studied. For an element with more than one isotope give the average atomic mass; it may also be useful to give the masses of the individual isotopes.
 - (iii) Half-life and mode of decay of a radioactive nuclide (but not necessarily a detailed decay scheme).
 - (iv) What neutron induced reactions are energetically possible in the energy range studied? (include Q values and threshold energies).
 - (v) If (n,n') is possible what excited states of the target nuclides will be formed, and what spin and parity values are involved? Can these be excited with s-wave neutrons incident and emergent?
 - (vi) Reasons if any why some of the possible neutron reaction cross-sections may be ignored. For example if the (n, α) reaction is energetically possible its cross-section may be negligible on account of the Coulomb barrier. Ideally the penetration factor should be given for the energy range studied (or for the maximum of the energy range) and an estimate of the order of magnitude of the cross-section.
 - (vii) Turning to the non-negligible neutron reactions, what experimental data are available for the cross-section, angular distributions and secondary neutron spectra? (include v , α , and η for fissile materials).
 - (viii) Discuss the derived resonance parameters. Note the resonance theory used and the method of analysis; and other assumptions or approximations. Try to find out if any of the experimenters ignored the factor $(A+1)^2 / A^2$ (see Appendix A).

- (ix) Are there shortcomings in the methods of measurement or discrepancies in the data?
- (x) Are the discrepancies adequately explained or explainable?
- (xi) Are the data consistent with theoretical expectations? (e.g. does σ_{nn} ($E = 0$) satisfy Wick's limit? do the resonance partial widths obey the Lane-Thomas-Wigner sum rule? see Appendices A and B).
- (xii) Tabulate preferred values for the cross-sections and/or the resonance parameters. If the cross-sections are to be calculated from the resonance parameters by the use of a computer programme it is essential to give values for all relevant parameters even if some have to be estimated or simply guessed; (i.e. Γ 's, nuclear radii, and compound nucleus spin and parity values). In using the recommended resonance parameters should one explicitly include the factor $(A+1)^2/A^2$ or should it be ignored? (see Appendix A).
- (xiii) Are the resonance parameters consistent with directly measured resonance integrals (if any)? In the case of capture and fission cross-sections integral comparisons are useful between the cross-section derived from resonance parameters and the differential cross-section directly measured with thin samples at a neutron spectrometer. Partial resonance integrals may be calculated over comparatively narrow energy intervals arbitrarily chosen. Comparisons may also be made with resonance integrals determined from integral measurements: allowance should be made for contributions due to unresolved resonances ($l = 0, 1, 2$).
- (xiv) Are the resonance parameters consistent with the known thermal capture and fission cross-sections and the free atom scattering cross-section? What can be said about the top negative energy resonance? Allowance should be made for the expected contributions of distant resonances at positive and negative energies.
- (xv) At what energies are resonances beginning to be lost for lack of resolution?
- (xvi) How should the cross-sections be determined in this region?
- (xvii) What resonance statistics are available for the unresolved resonance region? Strength functions and mean resonance spacing for given J and π . (If possible give strength functions for s, p, and d waves, or give some kind of rough theoretical estimate if reliable data are not available).
- (xviii) How does the observed mean spacing of resonances of given J and π compare with theoretical expectations?
- (xix) It could be of interest to illustrate the relative contributions of s, p, and d wave excitations to the mean cross-section; say to $\bar{\sigma}_y(E)$.

- (xx) Try to assign realistic uncertainties (standard error) to the preferred values of cross-sections, resonance parameters, etc. taking into account what the experimenters claimed and the actual discrepancies between different measurements. The idea should be to serve the users' interests - not to preserve unrealised or unrealistic claims of the experimenters.

(It is usually much more difficult to assess the uncertainties reliably than to select preferred values; on the other hand it may not merit very much time and effort).

- (xxi) What further experiments are needed, to resolve discrepancies, to improve accuracy if this is particularly low in any area, and to fill gaps in the experimental information?
- (xxii) Are there any problems which have been inadequately studied in this evaluation, for lack of time, or any new data since the tabulation was completed?
- (xxiii) Comparisons should be made with any other evaluations for the same material. In what ways is this new evaluation better than the older ones?
- (xxiv) Finally, an essential but obvious item, references should be given to all experimental and theoretical data which have been considered, or to some acceptable earlier review.

J. S. Story

1st December, 1964.

APPENDIX A

A well-known and typical resonance cross-section formula is

$$\sigma_{n\gamma}(E) = \pi \chi^2 \frac{\Gamma_n \Gamma_\gamma}{(E - E_\lambda)^2 + \Gamma^2/4} \quad (1)$$

The factor χ^2 relates to the motion in the centre-of-mass reference system. It is proportional to

$$\left(\frac{A+1}{A}\right)^2 \frac{1}{E}$$

where E is the neutron energy in the laboratory co-ordinate system and A is the atomic mass of the target atom in units of the neutron mass.

Experimenters often ignore this factor $(A+1)^2/A^2$ when deriving resonance parameters from their data.

When the spin state of the resonant state is unknown it is frequently assumed that $g = \frac{1}{2}$ when the neutron width is being evaluated. Then values given for Γ_n or Γ_n^0 may be more strictly the values of $2g\Gamma_n$ or $2g\Gamma_n^0$. This convention is used in BNL 325 (1958 and 1960) when J is unknown.

The energies and widths appearing in the final factor in (1) above are commonly represented in the laboratory frame of reference. The reduced width γ^2 appearing in theoretical arguments is referred to the centre of mass frame. It is related to the experimental partial width Γ by

$$2P \gamma^2 = \frac{A}{A+1} \Gamma$$

However, so far as the neutron width for the incident neutron is concerned note that the penetration factor P is given by

$$\frac{A}{A+1} \frac{\sqrt{2mE}}{\hbar} R v_1$$

where m is the neutron mass, and $v_0 = 1$, $v_1 = x^2/(1+x^2)$, etc:
 $x = kR$ is evaluated in the centre of mass frame.

Lane, Thomas & Wigner, Phys. Rev. 98, 693 (1955) give the following approximate sum-rule for the partial widths

$$\sum_{\lambda} (\gamma_{\lambda c})^2 \approx \frac{\hbar^2}{M_c (R_c)^2}$$

where M_c is the reduced mass in channel c and R_c is the effective radius. The summation extends over all levels λ excited in channel c within an energy interval comparable with the width of the single-particle giant resonances. In practice it is probably most convenient to regard the right-hand-side as a rough upper limit for a more restricted sum: for example the sum might be restricted to a single term, or it might be extended over all the resolved resonances excited in channel c .

APPENDIX B

Wick's inequality gives a theoretical lower limit to the differential elastic scattering cross-section at zero scattering angle

$$\left. \frac{d \sigma_{nn}(\theta)}{d\Omega} \right|_{\theta=0} \geq \left(\frac{k \sigma_T}{4\pi} \right)^2$$

where k is the wave number of the incident neutron in the centre of mass frame. Writing

$$\frac{d \sigma_{nn}(\theta)}{d\Omega} = \sigma_{nn} \cdot p(\cos \theta) / 2\pi \int_{-1}^{+1} p(\cos \vartheta) d\cos \vartheta$$

where the first factor on the right is the integrated elastic scattering cross-section, Wick's inequality implies that

$$\frac{p(\cos \theta = +1)}{\int_{-1}^{+1} p(\cos \vartheta) d\cos \vartheta} \geq (0.192024 \pm 0.000028) \left(\frac{A}{A+1} \right)^2 E \sigma_T^2 / \sigma_{nn}$$

with E in MeV, and the cross-sections in barns.